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Numerical Simulation of High Quark Densities in QCD with two Colours

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The DESY-Swansea Collaboration performed numerical simulations investigating SU(2) lattice gauge theory at non-zero chemical potential with one staggered quark flavour in the adjoint representation. This lattice model has similar features to QCD itself and its study gives interesting insights into some open problems of high density quark matter. In particular the rôle of the "sign problem" can be clarified in connection with diquark condensation and the phase diagram.

1 Introduction

The fundamental theory of strongly interacting matter is Quantum Chromo-Dynamics (QCD), which is a relativistic quantum field theory with quarks and gluons as quanta of the elementary constituent fields. Physical properties of strongly interacting matter, manifested in high energy heavy ion collisions, in the early Universe or in neutron stars, can, in principle, all be deduced from this theory. An important calculational method in QCD is numerical Monte Carlo simulation on space-time lattices.

In recent years, significant progress has been made in understanding the phase diagram of QCD at high quark- (or baryon-) number density. On the basis of model calculations[1,2], it is now believed that the ground state of QCD at high density and low temperatures is characterised by a diquark condensate which spontaneously breaks gauge and/or baryon number symmetries (for recent reviews see[3]). This leads to phenomena such as *colour superconductivity* and/or *colour-flavour locking* which have substantial influence on the physics of high density hadronic (quark-) matter and have a major impact, for instance, on the properties of heavy neutron star cores. However, although the results appear to be qualitatively independent of the specific model and approximation employed, little can be said quantitatively due to the lack of a first-principles, non-perturbative method that can access the relevant regions of the phase diagram.

Non-perturbative Monte Carlo simulations in lattice QCD, which are first-principles methods, fail when a chemical potential term μn_B, where n_B is the quark number density, is added to the Lagrangian. The reason is that the Euclidean-space fermion determinant becomes complex. As a consequence, standard simulation algorithms cannot be applied. However, it is possible to study QCD-like theories where the fermion determinant remains real even at non-zero μ. These theories can be used as testbeds to examine the validity of the models used to study real QCD, as well as directly to improve our understanding of phenomena such as diquark condensation and phase transitions in dense matter. Examples of such theories with real quark determinant are two-colour (SU(2) colour) QCD and QCD with adjoint quarks.

The DESY-Swansea Collaboration studied two-colour QCD with staggered quarks in the adjoint representation[4–6]. The use of a particular lattice fermion formulation (with staggered fermions) is important because for real or pseudoreal representations of the gauge group the pattern of symmetry breaking is expected to be different in the continuum and at non-zero lattice spacing[7]. In this QCD-like model it is possible to investigate several interesting questions. Its basic features are:

- For an odd number of staggered flavours N, the fermion determinant may be negative. This means that this model has a *sign problem*, which may make simulations at large μ difficult. At the same time a sign is simpler than the continuum of phases in QCD. It may thus be feasible to make progress using standard means, or at least expose physical distinctions between the positive and negative sectors.

- For zero quark mass (m) and vanishing chemical potential $m = \mu = 0$ the $\mathrm{U}(N) \times \mathrm{U}(N)$ flavour symmetry is enhanced to a $\mathrm{U}(2N)$ symmetry which relates quarks to antiquarks. This symmetry is broken by the chiral condensate, leaving $N(2N-1)$ massless Goldstone modes, which become degenerate pseudo-Goldstone states for $m \neq 0$.

- When $N \geq 2$ these pseudo-Goldstone states include gauge invariant scalar diquarks which, though degenerate with the pion at $\mu = 0$, carry baryon number. These models with $N \geq 2$ can be studied for $\mu \neq 0$ by chiral perturbation theory (χPT)[8]. The main result is that for $\mu > m_\pi/2$, where m_π is the pion mass, the chiral condensate rotates into a diquark condensate (the two being related by a $\mathrm{U}(2N)$ rotation) while the baryon density increases from zero.

- The model with $N = 1$ is not expected to contain any diquark pseudo-Goldstones and is not accessible to χPT. One expects an onset transition as some $\mu_o \approx m_b/n_q > m_\pi/2$, where m_b is the mass of the lightest baryon and n_q its baryon charge.

- For $N = 1$ the gauge invariant scalar diquark operator is forbidden by the Pauli Exclusion Principle; there is, however, a possibility of a gauge non-singlet, and hence colour superconducting, diquark condensate at large chemical potential.

The numerical simulation of lattice gauge theories is performed on a hypercubic lattice in four dimensional Euclidean space. The fourth coordinate, besides the three space coordinates, is imaginary time. In the path integral formulation the Euclidean action is needed which gives the weight of lattice field configurations. For the gauge field part the standard Wilson action, weighted by the inverse gauge coupling β, is taken[9]. The fermionic part of the lattice action, with quark mass m and chemical potential of quark charge μ, can be defined as follows:

$$\begin{aligned} S &= \sum_{x,y} \bar{\chi}^p(x) D_{x,y}[U,\mu] \chi^p(y) + m \bar{\chi}^p(x) \delta_{x,y} \chi^p(y) \\ &\equiv \sum_{x,y} \bar{\chi}^p(x) M_{x,y}[U,\mu] \chi^p(y), \end{aligned} \tag{1}$$

where the index p runs over N flavours of staggered quark, and D is given by

$$D_{x,y} = \frac{1}{2}\sum_{\nu\neq 0}\eta_\nu(x)\left(U_\nu(x)\delta_{x,y-\hat{\nu}} - U_\nu^\dagger(y)\delta_{x,y+\hat{\nu}}\right) + \frac{1}{2}\eta_0(x)\left(e^\mu U_0(x)\delta_{x,y-\hat{0}} - e^{-\mu}U_0^\dagger(y)\delta_{x,y+\hat{0}}\right). \quad (2)$$

The $\chi, \bar{\chi}$ are single spin component Grassmann objects, and the phases $\eta_\mu(x)$ are defined to be $(-1)^{x_0+\cdots+x_{\mu-1}}$. The link matrices in the adjoint representation U_μ are real 3×3 orthogonal matrices. The Grassmann variables in the path integral can be integrated out, resulting in the determinant of the fermion matrix M appearing in (1). This *fermion determinant* takes into account the effects of virtual fermion-antifermion pairs on the gauge field.

The main difficulty in numerical simulations of gauge theories with fermions is to include the fermion determinant. We have used two different simulation algorithms, the hybrid Monte Carlo (HMC) algorithm[10] which is the standard choice for QCD, and a Two-Step Multi-Bosonic (TSMB) algorithm[11] which has been developed recently in connection with a study of supersymmetric Yang-Mills theory.

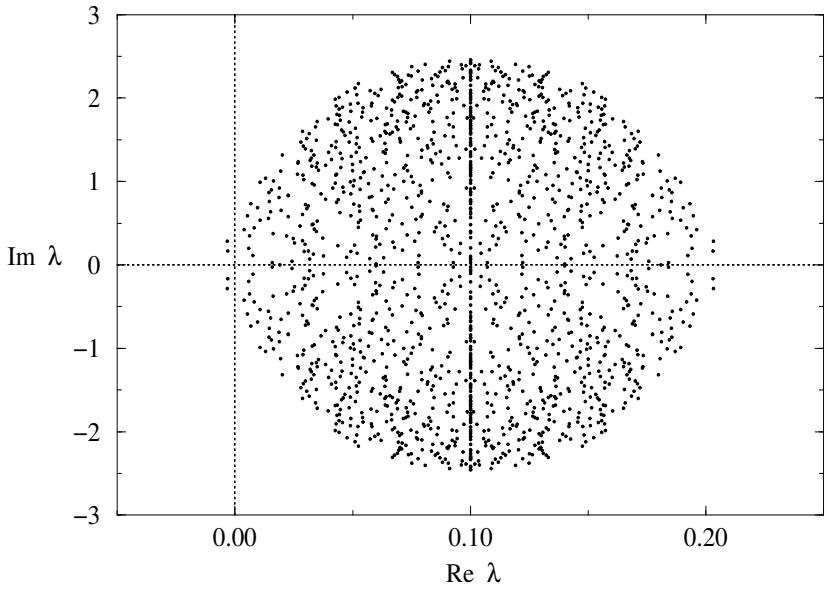

Figure 1. *Typical eigenvalue spectrum of the fermion matrix on a* $4^3\cdot 8$ *lattice at (*$\beta = 2.0,\ m = 0.1,\ \mu = 0.35$*).*

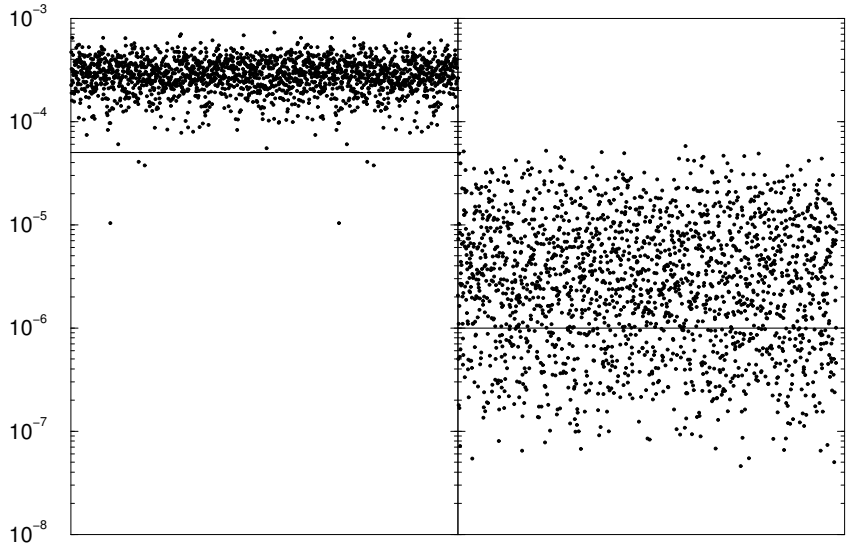

Figure 2. *The lowest eigenvalues of the hermitean fermion matrix, for $\mu = 0.3$ (left) and $\mu = 0.4$ (right). The lines indicate the lower bound ϵ of the polynomial approximation employed.*

2 The Sign of the Determinant

At zero chemical potential $\mu = 0$ the complex eigenvalues of the fermion matrix M in (1) lie on a line parallel to the imaginary axis with real part equal to the quark mass $\mathrm{Re}\lambda = m$. Since the eigenvalues come in complex conjugate pairs, the determinant of the fermion matrix at $\mu = 0,\ m > 0$ is positive. After introducing a non-zero chemical potential the eigenvalues spread out into an elliptical region of the complex plane (see, for instance, figure 1).

At large enough chemical potential the region occupied by the eigenvalues of the fermion matrix reaches the origin of the complex plane (this is actually the situation in figure 1), which has important consequences for the behaviour of the system. From the technical point of view this is manifested by the appearence of very small eigenvalues of the squared fermion matrix (see figure 2), which makes the numerical simulation difficult. The very small eigenvalues occur because there are sign changes of the fermion determinant. It turns out that this can only be seen in the TSMB simulation because the HMC algorithm is based on small steps in configuration space and cannot in practice change the determinant sign. This is an important observation showing that under these circumstances the standard HMC algorithm is not applicable because it is not ergodic. As we shall see below, the HMC simulation is very similar to the restriction of the TSMB simulation to the positive determinant sector. The omission of the gauge configurations with negative determinants has important consequences for the physical results.

In simulations with the TSMB algorithm the qualitative change for increasing chemical potential can also be clearly seen in the distribution of the *reweighting factors* (see figure 3). These are required because the polynomial approximations applied in this algorithm[12] are not exact near zero eigenvalues. The reweighting factors, which also include the sign

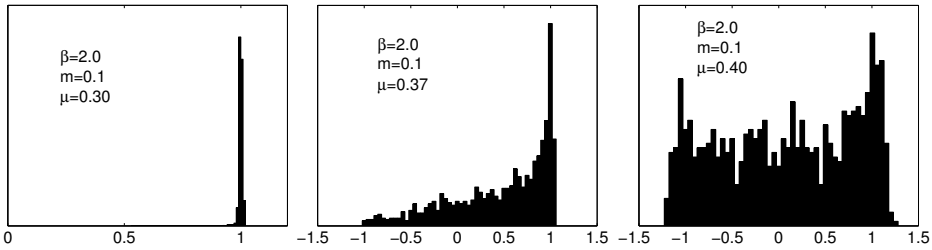

Figure 3. *Reweighting factors, for $\mu = 0.3$ (left), $\mu = 0.37$ (middle) and $\mu = 0.4$ (right). As the proportion of negative determinant configurations increases, the preferred distribution of reweighting factors changes from being sharply peaked around 1 to nearly flat. The polynomial orders (n_1, n_2) are (48,500), (80,800) and (100,1000) respectively.*

of the fermion determinant, are correcting for this. As it can be seen in figure 3, the reweighting factors are strongly peaked near 1 for a μ value where the spectrum does not yet touch zero ($\mu = 0.3$). At $\mu = 0.37$, where the spectrum just reaches the origin, some configurations with negative reweighting factor (i.e. negative determinant) start to appear. Finally, at $\mu = 0.4$ the frequency of both signs is already almost equal and the sign problem is serious.

3 Simulation Results

Having a suitable simulation algorithm (TSMB) which samples both positive and negative determinant sectors properly one can compare results with and without taking into account the determinant sign. Most of the results of the DESY-Swansea Collaboration have been obtained at $\beta = 2.0,\ m = 0.1$ on a $4^3 \cdot 8$ lattice[4–6]. It turned out that the results in the positive sector of the TSMB simulations are close to the HMC simulation results and both are qualitatively similar to the results of chiral perturbation theory for theories with diquark Goldstone modes (for instance, $N = 2$ flavours)[8]. This is not surprising because taking the absolute value of the fermion determinant in the path integral measure is equivalent to consider $\sqrt{\det(M^\dagger M)}$ instead of $\det(M)$. An example of the good agreement between the results of HMC simulations and chiral perturbation theory predictions is shown by figure 4 in case of the chiral condensate $\langle\bar{\psi}\psi\rangle$.

The inclusion of the fermion determinant sign, in the single staggered flavour ($N = 1$) model we are interested in, changes the physical results qualitatively. The main effect is that the phase transition at chemical potential $\mu \simeq \frac{1}{2}m_\pi$, which is signalled for instance by the sharp drop of the chiral condensate in figure 4, disappears due to a cancellation between the contributions of positive and negative sectors. As an example one can consider the behaviour of the quark density shown in figure 5. The increase beyond $\mu = 0.35$ disappears once the signs are taken into account properly. Unfortunately, the severe sign problem does not allow us to go much beyond $\mu = 0.4$ where the onset phase transition of the $N = 1$ model is expected.

A natural explanation of the agreement between the HMC and positive determinant results and χPT predictions is that the positive determinant sector mimics a theory with two flavours: one quark and one 'conjugate quark'[13]. We may cast further light on this by

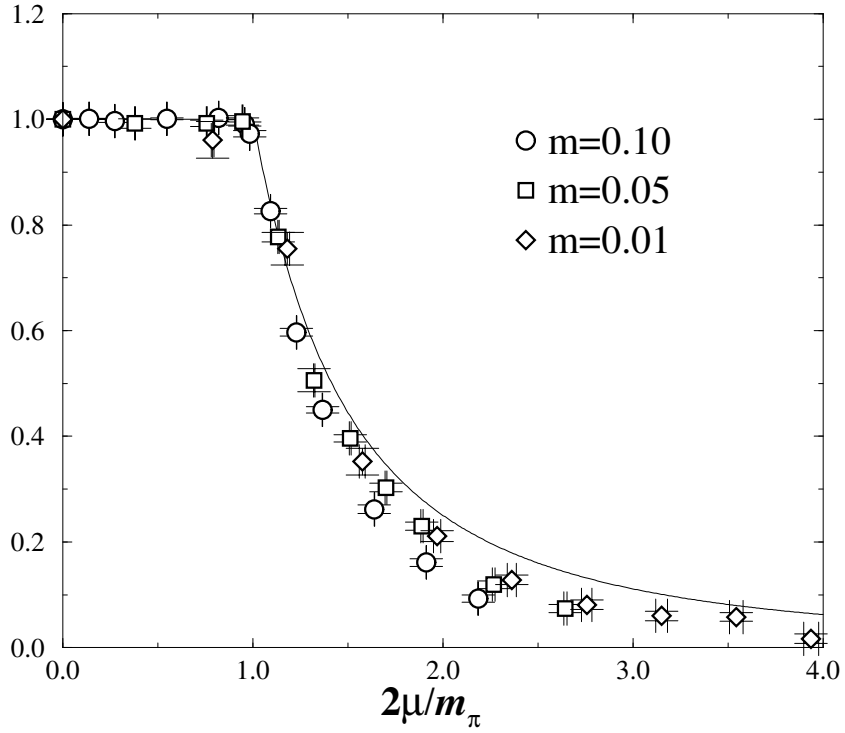

Figure 4. *Rescaled chiral condensate vs. chemical potential obtained in HMC simulations together with the χPT predictions.*

studying the behaviour of the diquark condensate of the $N = 2$ diquark operator

$$qq_{\mathbf{3}} = \frac{i}{2}\left[\chi^{p\,tr}(x)\varepsilon^{pq}\chi^{q}(x) + \bar{\chi}^{p}(x)\varepsilon^{pq}\bar{\chi}^{q\,tr}(x)\right], \tag{3}$$

where $p, q = 1, 2$ are explicit flavour indices and ε the antisymmetric tensor. A non-zero expectation value $\langle qq_{\mathbf{3}}\rangle \neq 0$ is expected in the two-flavour theory, violating the symmetry of the Lagrangian under global U(1) baryon number rotations. Physically this implies a superfluid ground state and (via Goldstone's theorem) exactly massless scalar excitations. This accounts for the proliferation of small eigenvalues observed in section 2. The superfluid condensate may be determined by introducing a diquark source term in the action, which now describes two flavours,

$$S[j] = S + j\sum_{x} qq_{\mathbf{3}}(x)\,. \tag{4}$$

One has to extract the condensate $\langle qq_{\mathbf{3}}(j)\rangle = V^{-1}\partial \ln Z[j]/\partial j$, and extrapolate the results to $j = 0$[14]. The HMC simulations do support $\langle qq_{\mathbf{3}}\rangle \neq 0$ for $\mu \geq m_\pi$, as expected. In the TSMB simulations taking into account the determinant sign the diquark condensate $\langle qq_{\mathbf{3}}\rangle$ is suppressed.

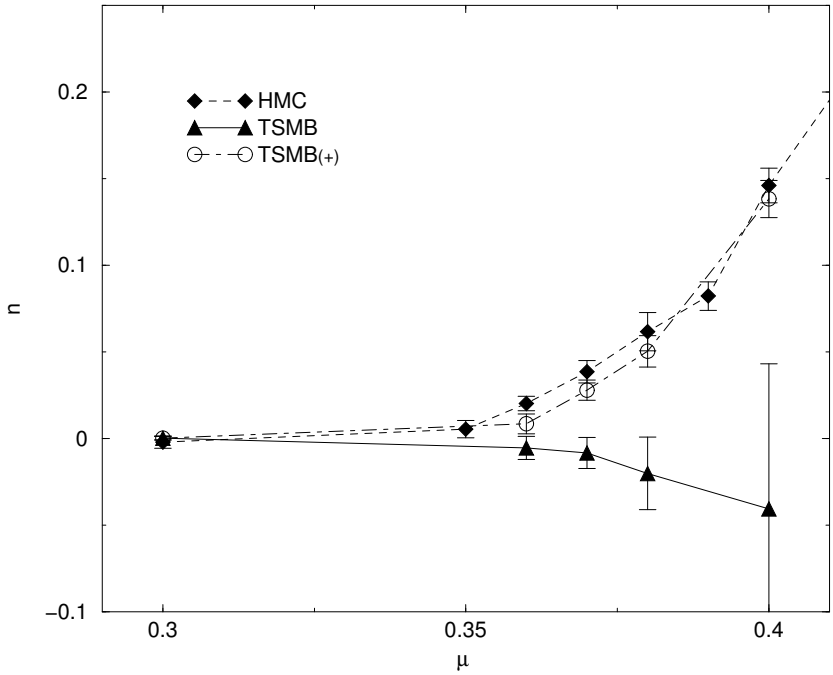

Figure 5. *The fermion density from TSMB and HMC simulations. In case of TSM simulations the result in the positive determinant sector is shown separately (open symbols).*

4 Conclusions

We have studied two-colour QCD with one flavour of staggered quark in the adjoint representation. We have employed two different simulation algorithms, and have gained insight into the optimal tuning of the TSMB algorithm in the high density regime. This is the preferred algorithm not only because it is capable of maintaining ergodicity via its ability to change the determinant sign, but also because it more effectively samples small eigenmodes, which are important in the presence of a physical Goldstone excitation. We find that the positive determinant sector behaves like a two-flavour model, and exhibits good agreement with chiral perturbation theory predictions for such a model. At higher chemical potentials there are some indications of a breakdown of χPT, and possible signs of a further phase transition. However, data from larger volumes and smaller bare quark masses would be needed to make these observations definitive.

Above the onset transition in the positive determinant sector, we have successfully obtained a signal for a non-zero two-flavour diquark condensate $\langle qq_{\mathbf{3}}\rangle$, indicating a superfluid ground state for $\mu > m_\pi/2$. The chiral condensate rotates into this diquark condensate, in good quantitative agreement with the behaviour predicted by χPT. This feature also enabled us to achieve reasonable control over the necessary $j \to 0$ extrapolation[6].

When the negative determinant configurations are included in the measurement, the onset transition and diquark condensation disappear. This is what we would expect for the one-flavour model and is consistent with the Pauli Exclusion Principle. There is a

strong evidence for this scenario, providing a conclusive demonstration, should any still be needed, that the determinant sign plays a decisive role in determining the ground state of systems with $\mu \neq 0$. Unfortunately, the severity of the sign problem means we have not been able to locate the real onset transition for this model.

The numerical calculations presented in this report have been performed on the Cray T3E of the NIC, Jülich since 1999. The total CPU time was about 180.000 hours.

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